OAK RIDGE NATIONAL LABORATORY
Transportation Program

Fiscal Year 2005 Transportation Program Highlights

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Introduction

The Oak Ridge National Laboratory (ORNL) Transportation Program supports the mission of the FreedomCAR and Vehicle Technologies (FCVT) Program, a part of the Department of Energy's (DOE's), Office of Energy Efficiency and Renewable Energy (EERE). The Program aims to develop more energy-efficient and environmentally friendly highway transportation technologies that enable America to reduce petroleum usage. ORNL conducts pre-competitive research and development (R&D) on a wide range of technologies, including 1) advanced combustion regimes in vehicle engines; 2) the effects of fuel properties on engine efficiency and emissions; 3) power electronics and electric machines; and 4) advanced materials that are strong, lightweight, and durable.

The Program supplements in-house expertise and facilities through subcontracts with private industry and universities to provide specialized analysis, equipment, technical services, and so forth. In addition, partnerships with industry are an important part of developing transportation technologies. Partnerships are executed through a variety of mechanisms, including Cooperative Research and Development Agreements (CRADAs), user agreements, and cost-shared subcontracts. These partnerships ensure that ORNL's R&D activities address the technical barriers faced by industry, such as creating advanced technology components and vehicles that offer increased fuel efficiency and meet 2007 and 2010 Environmental Protection Agency (EPA) emission standards. The Transportation Program also addresses the longer-term national goals of decreasing and eventually eliminating dependency on imported oil in the transportation sector. ORNL R&D activities in power electronics and energy storage are applicable to hybrid and plug-in electric vehicles in the short term and fuel cell-powered automobiles in the long term. Projects to develop clean, efficient diesel engines and diesel exhaust aftertreatment systems enable the use of fuel-efficient diesel engines in light-duty vehicles. Such projects also contribute to 21st Century Truck Partnership (21st CTP) goals to increase efficiency, reduce emissions, and improve safety and economy in medium and heavy-duty trucks. Materials R&D projects support and enable the development of these innovative technologies for both light-duty and heavy-duty vehicle applications.

ORNL's Transportation Program received approximately $41.5 million in new budget authority in fiscal year (FY) 2005. The Program expended $11 million in R&D subcontracts, much of which was supplemented by substantive cost sharing. The Program supported approximately 190 full time-equivalent ORNL scientific and technical staff, and two national user facilities: the National Transportation Research Center (NTRC) and the High Temperature Materials Laboratory (HTML). This research resulted in over 300 presentations and publications, and 20 patent disclosures. During FY 2005, 11 patents were awarded as a result of earlier disclosures.

In FY 2005, Edmund T. Grostick served as the ORNL Transportation Program's Acting Program Director. During Mr. Grostick's time with the Program, the ORNL Transportation Program attained its first "outstanding" performance rating from DOE. In July 2005, Mr. Grostick retired from this position and was succeeded by Dr. Raymond G. Boeman as Transportation Program

Director. Dr. Boeman received his PhD in Engineering Mechanics from Virginia Polytechnic Institute and State University in 1990. Since joining ORNL in January 1991, Dr. Boeman has played a vital role in transportation research. After successfully managing an automotive adhesives research project at ORNL, Dr. Boeman took a one-year assignment in Detroit, MI, to work with the Automotive Composites Consortium. This one-year assignment turned into five years of working hand-in-hand with U.S. automakers. In the spring of 2004, Dr. Boeman accepted a new assignment with DOE in Washington, DC, providing technical assistance to the 21st CTP through the FCVT Program. After the completion of this assignment, Dr. Boeman has returned to ORNL and taken over management of the Transportation Program. His experience with industry and DOE will be a tremendous asset for the Program.

This report is organized in two sections: 1) Project Summaries and 2) Technical Highlights. The Project Summaries section provides brief overviews of the Transportation Program's activities in FY 2005. The Technical Highlights section includes detailed descriptions of noteworthy research results and technical achievements.

Project Summaries

National Transportation Research Center

In the last quarter of FY 2005, NTRC emphasized establishing a user base to increase the number of user agreements for the Test Machine for Automotive Crashworthiness (TMAC). A TMAC information package was assembled, potential TMAC users were contacted, and a targeted development effort was mounted within the ACC Energy Management group. Proposals from user candidates are expected in FY 2006 as a result.

In FY 2005, three organizations inquired about establishing user agreements with NTRC, but none resulted in a signed user agreement. A heavy vehicle dynamics and rollover project was completed, bringing ORNL together with Dana, Michelin, and National Transportation Research Center, Inc. (NTRCI). The project studied vehicle rollover characteristics of a conventional tractor/box trailer configuration, first using dual tires and then substituting next-generation single tires. Results showed a stability improvement with the next-generation single tires. A paper was submitted to the International Truck and Bus Safety and Security Symposium and was subsequently selected as one of four outstanding symposium papers. This successful industry-laboratory relationship contributed to the formation of an outstanding team that included ORNL and Dana in an FCVT-funded FY 2005 heavy-duty cycle project. The project will extend through FY 2006 and involves instrumenting a heavy-duty tractor and trailer combination. The instrumentation will collect data on characteristics such as fuel usage, engine operating parameters, emissions stability, and other details (e.g., weather conditions) related to the long-haul driving environment. The data will be used in computer models that can be used by engineers, designers and manufacturers to develop heavy-duty vehicles that are lighter, safer, more fuel-efficient, and friendlier to the environment.

Planning and negotiation continued for the development of a new facility co-located with NTRC. This facility, which will be called the Energy Conversion Research Facility (ECRF), would primarily provide additional analytical and engine test cell space for the Fuels, Engines, and Emissions Research Center (FEERC); facilities for alternative liquid and gaseous fuels R&D; facilities for distributed energy power plant R&D; and bench-scale analytic and experimental facilities for fuel cell R&D. The envisioned facility will be about 31,000 square feet. Just over half will be dedicated to research space and the remaining to research support. Similar to NTRC, ECRF is expected to be built by or leased from a private third party. The facility could be ready for occupancy as early as FY 2007.

The ORNL Business Management Division has calculated the FY 2005 cost savings derived from housing researchers at NTRC rather than on the main ORNL campus to be approximately $987,000, for a cumulative savings (FY 2002-2005) of approximately $3,783,400.

High Temperature Materials Laboratory

In FY 2005, the High Temperature Materials Laboratory (HTML) User Program received a record high of 110 user proposals. Of these, 21 were from first-time user institutions, and the number of user agreements with ORNL increased from previous years with 33 new agreements signed (27 from industrial concerns and six from colleges and universities).

The sub-angstrom resolution electron microscope [Aberration Corrected Electron Microscope (ACEM)] became functional in FY 2005. With the ability to exhibit single-atom resolution, the ACEM was used on several FCVT-sponsored projects on prototypical catalyst materials (i.e., atoms atomically-dispersed on an alumina substrate). Other HTML user projects and FCVT-sponsored projects have been accepted for future work using the ACEM.

Improvements to the Neutron Residual Stress Facility (NRSF-2) were completed in FY 2005, and related user projects were initiated. As one of the first users of the facility, Caterpillar investigated a new welding procedure. The procedure promised to be more rapid and less costly than the current one in use, but Caterpillar needed to know if it produced the same or less residual stress. Caterpillar used the NRSF-2 facilities to measure the residual stress. The new NRSF-2 has a higher number of detectors, a faster response time, a higher neutron flux on the sample, more robust specimen holders (capable of supporting hundreds of kilograms), and more flexibility. The facility also houses a furnace, mechanical testing stage, and atmospheric control capability. These improvements to NRSF-2 have made it a unique, world-class facility.

With the Spallation Neutron Source (SNS) nearing completion, HTML moved forward in its plans for the VULCAN “engineering materials diffractometer” (located at SNS). In FY 2005, HTML was able to 1) provide staff support to the SNS-VULCAN instrument development team, 2) design and build an off-spectrometer specimen alignment system, and 3) procure additional detectors.

Of the 110 proposals received in FY 2005, 38 were on subjects directly relevant to FCVT. These included projects in areas such as aluminum and aluminum matrix composites, magnesium and its composites, high-strength steels, diesel particulate filters, exhaust emission catalysts, and both hydrogen-internal combustion engine (ICE) and diesel engine fuel injector components. Thirteen projects were not directly relevant to FCVT but did involve transportation-related projects such as welding and weld structural quality examination, metal casting, spark plug development, new high-strength bulk metallic glasses, and thermal properties of engine coolant additives. Other projects (39) were relevant to other EERE topics like hydrogen storage, hydrogen membranes, fuel cells, and even solar cell materials. In addition, 34 projects were relevant to other areas, including high-speed or high-power electronic materials and components, titanium alloys for medical implants, catalysts for bioprocessing, and numerous basic research projects on nanomaterials.

Advanced Power Electronics

ORNL's Power Electronics and Electric Machinery Research Center (PEEMRC) at NTRC conducts high-risk, long-term research, evaluates hardware, and provides technical support to the FCVT Program's Advanced Power Electronics and Electric Machines (APEEM) activity. Through PEEMRC, ORNL serves on the FreedomCAR Electrical and Electronics Technical Team. ORNL researchers evaluate technical proposals for DOE and lend their technological expertise to the evaluation of projects and developing technologies. ORNL executes specific projects for DOE in power electronics, electric machines, and thermal control, in order to help remove technical and cost barriers so that technologies will be suitable for use in advanced vehicles that meet the goals of FCVT. This provides a portfolio of options that automotive manufacturers and suppliers can use when developing their unique solutions for hybrid and fuel cell vehicles.

Significant progress was made in FY 2005 in the development of advanced electric machines and power electronics components for hybrid electric vehicles (HEVs) and fuel cell–powered vehicles. A prototype radial gap interior permanent magnet motor with external field excitation was built. Test results showed a doubling of the torque at the same full-load current. Additionally, it can increase the motor's speed range and provide both field weakening and enhancement. Testing of the prototype successfully demonstrated the field weakening and enhancement features of this concept.

An integrated DC-DC converter topology was also built and tested by ORNL. The technology employs only four switches while providing a triple voltage bus (14 V/42 V/high voltage). The integrated converter should provide greater reliability, reduced cost, and reduced size, while providing the multiple voltages required by HEVs and fuel cell vehicles. Further cost savings are realized by eliminating the inductor. Simulation studies verified the functionality of the topology and indicated an operating efficiency of 93 percent between 30 and 70 percent of full load. A 2-kW prototype was fabricated and functional testing proved the concept.

ORNL developed an integrated traction and compressor drive system which shares components for the two functions. For the compressor drive, the number of inverter components, including semiconductor switches and gate drive circuits, were reduced by more than one-third. The compressor drive control was incorporated into the traction motor controller, rather than having a separate control circuit, further reducing the cost. ORNL tested a prototype inverter with a three-phase induction motor and a two-phase compressor motor. These tests demonstrated that the inverter concept can drive either motor separately or both motors simultaneously without affecting the other's operation.

Additionally in FY 2005, a novel thermal control system was developed by ORNL. This concept uses refrigerant from the vehicle air conditioning system to provide thermal control for an inverter and motor specifically designed to use this coolant. Because this coolant system integrates with the high-temperature side of the vehicle's air conditioning (A/C) system, it does not use the compressor and results in a coefficient of performance (COP) of 30 or greater. A prototype system was designed and fabricated using an automotive A/C system. System integration issues associated with refrigerant migration and system dynamic performance were resolved and design activities were initiated for the motor and inverter. Heat transfer studies demonstrated a heat flux in excess of 150 W/cm^2. By efficiently cooling the inverter and motor, it will be possible to reduce the size of the inverter by two-thirds.

Fuels, Engines, and Emissions

ORNL's Fuels, Engines, and Emissions Research Center (FEERC), located at NTRC, conducted R&D for multiple subprograms of the FCVT Program in FY 2005, including Advanced Combustion and Engine R&D, Fuels Technology, and Vehicle Systems. Through FEERC, ORNL has collaborated with industry through five CRADAs in engine/emissions technology, as well as through less-formal, but very active collaborations with approximately 15 additional private companies and non-DOE agencies. Several of the CRADAs have resulted in the installation of unique research hardware at FEERC. In addition, six private sector firms sponsored R&D at the center in FY 2005. FEERC held its third Guidance and Evaluation Panel meeting in November 2004, with members from Ford, Cummins, BP-Amoco, Caterpillar, Umicore, and others.

Researchers at FEERC are highly engaged in supporting FreedomCAR and Fuel Partnership and 21st CTP programmatic activities, including the Advanced Combustion and Emission Control Technical Team, the Diesel Crosscut Team, and the 21st CTP Lab Council. ORNL provides co-leadership with industry through the Crosscut Lean Exhaust Emissions Reduction Simulation (CLEERS) activity. In fuels technology, FEERC staff members co-chair three subteams of the Advanced Petroleum Based Fuels-Diesel Emission Control project and sit on the steering committee in partnership with the National Renewable Energy Laboratory (NREL). Researchers at FEERC also participate in working groups for the Coordinating Research Council. FEERC staff and facilities play significant roles in the Advanced Reciprocating Engine Systems (ARES) projects in the Distributed Energy Program. Both FCVT and ARES benefit from this leveraging.

In FY 2005, there were a number of additions to capabilities at FEERC in order to stay current with the challenges and research requirements of the Center's partners and DOE. These include:

- A variable compression ratio engine was developed for ORNL;
- A unique, camless diesel research engine from CRADA partner International Truck and Engine Corporation; and
- Hydrogen fuel capability was added for engine and nitrogen oxides (NO_x) aftertreatment studies.

Advanced combustion engines research is undergoing an orderly shift to more emphasis on improving engine fuel economy through advanced combustion regimes and other technologies, while retaining critical projects on key remaining issues in emission controls.

ORNL participates with 14 other organizations in a Memorandum of Understanding (MOU) on Advanced Engine Combustion Research. ORNL's specific roles in the MOU are: 1) determining how advanced combustion regimes might be exploited for inherent efficiency gains; 2) determining the detailed emissions species generated by these combustion regimes; and 3) researching control strategies for full power density and transitions. Powerful capabilities in engine electronic control prototyping were exercised to show quick and near-seamless transitions between operating points within the low-temperature combustion (LTC) operating environment.

Although most LTC emphasis has been based on diesel fuel, gasoline-based homogeneous charge compression ignition (HCCI) engines can potentially yield higher efficiency than conventional spark-ignition engines and can also reduce emissions. ORNL has been studying the use of spark augmentation for stabilizing the cycle-to-cycle efficiency variation encountered in certain types of mixed-mode (conventional and HCCI) engines. Researchers have found that the cyclic dispersion encountered during the conventional-to-HCCI operation transition is complex (high period or deterministic chaos with noise) but is short-time predictable. This indicates that it may be possible to develop proactive control algorithms for stabilizing HCCI and for these transitions, helping expand the overall operating range.

Research on improving the efficiency of lean nitrogen oxide (NO_x) trap (LNT) regeneration led to a new strategy that integrated the features (low NO_x and high hydrocarbon)] of LTC with mild fuel enrichment to de-NO_x the LNT. The technique provides five to ten times the NO_x reduction per unit of excess fuel.

An engine management strategy was identified that can produce moderate levels of hydrogen in the engine exhaust in overall lean operation that would enhance the performance of lean-NO_x catalysts. The experiments to confirm this were requested by an automobile OEM.

The CLEERS team continued development and validation of a standard protocol for LNTs. The success of the LNT collaboration has provided a framework for similar data sharing and collaborations among CLEERS team members for urea-SCR (selective catalytic reduction) and diesel particle filter technologies. The team also maintained the website (http://www.cleers.org) and organized the eighth CLEERS workshop.

An extensive study of fuel property effects on both gasoline-based and diesel-based HCCI performance and emissions was completed. Results were published showing that the fuel properties could in fact expand or shrink the HCCI operating space in the case of gasoline fuels. For diesel-like fuels, the results show how the cool-flame reactions are prominent in fuels with a high cetane number. To more globally facilitate and coordinate research in this area, ORNL conceived a vision to initiate a comprehensive project on how fuel properties affect advanced combustion processes like HCCI. ORNL teamed with NREL to move the project plans forward. The effort will begin with design of a research fuel matrix via a working group of experts in this field convened under the auspices of the Coordinating Research Council. This project has been named FACE (fuels for advanced combustion engines).

ORNL supports the FCVT Vehicle Systems Team in cost modeling for advanced vehicle components, and in developing performance/emissions models for engine and exhaust aftertreatment components. In FY 2005, the efforts were redirected to aid the development of the Powertrain Systems Analysis Toolkit (PSAT) code in conjunction with Argonne National Laboratory (ANL). Johney Green, FEERC group leader, has been appointed to the FreedomCAR Systems Technical Team and is serving as a liaison to the Advanced Combustion and Emission Control Technical Team.

FEERC also contributed to FCVT's Environmental Impacts and Health Impacts activities in FY 2005 by assisting in the determination of the potential adverse impacts of new FCVT technologies being developed. The Watt Road Environmental Laboratory received FY 2005 funding from the FCVT Health Impacts activity for real-world truck emissions studies. Department of Transportation (DOT) and EPA have co-sponsored certain studies at the Watt Road laboratory. Ambient sampling of particulate matter and formaldehyde near the truck stop that is included in the field laboratory site has shown a strong variation throughout the day and dependence on ambient conditions. In-cab emissions sampling has been provided to show the impact of nearby idling trucks versus the in-cab levels just from idling the subject truck.

For FY 2006 and beyond, FEERC expects to continue activities in the combustion MOU with increased emphasis on engine efficiency improvements. In fuel technologies, matching fuel properties to advanced combustion will be addressed in the FACE project. In parallel, the critical remaining issues in emission controls must be addressed. CLEERS is expected to remain a focal point of those efforts.

Automotive Lightweighting Materials

ORNL supports the FCVT Program's Automotive Lightweighting Materials (ALM) activity by focusing on structural materials for vehicle body and chassis applications. ORNL looks specifically at those materials which have the potential to significantly reduce the weight of passenger vehicles without compromising vehicle lifecycle cost, performance, safety or recyclability. ALM's goals include developing and validating advanced material technologies by 2012 that, if implemented in high volume, could cost-effectively reduce the weight of body and chassis components by at least 60 percent with performance, reliability and safety characteristics comparable to those of conventional vehicle materials. ORNL conducts R&D activities in ALM research areas such as cost reduction, design data and modeling, manufacturability, tooling and prototyping, joining and assembly, performance enhancement, and maintenance. Efforts are further organized into activities in automotive metals, polymer composites, low cost carbon fiber, materials joining, non-destructive evaluation, and enabling technologies.

In FY 2005, ORNL demonstrated substantial progress in carbon fiber reinforced polymer matrix composites. Because of their high stiffness and strength, these composites offer to potentially reduce vehicle weight by more than 50 percent. The current barrier, however, to implementing these in automotive systems, is the cost of carbon fiber. During the past few years, the Program has been developing technologies aimed at reducing the cost of carbon fiber by focusing on both the raw materials and the processing methods being used. The Program is developing methods to rapidly and inexpensively stabilize, oxidize, carbonize, graphitize, and post-treat commercial grade carbon fibers, as well as using lower-cost starting materials.

In order to commercialize these technologies, they must first be merged into a single processing line that allows the application of a user-selected number of the new technologies with conventional processing technologies. The integration line, which is currently under development, will allow manufacturers to pick and choose which of the new technologies they wish to employ and resolve interface issues between conventional and advanced technologies prior to the design of new commercial lines. The program has established and brought the conventional part of the processing line to full operation and has designed and built the first full-scale unit of the advanced technology line.

Additionally in FY 2005, ORNL developed new experiments for the characterization of progressive crush of Advanced High Strength Steels (AHSS). New developments in AHSS metallurgy and processing, combined with computer and modeling advancements, require accurate material characterization and verified models in order to fully utilize the increased strengths of the materials. The TMAC was used to provide high quality component level data for development of material and structural computer models. Validated models were distributed to steel manufacturers and automotive designers and enable more accurate modeling and design of lightweight crashworthy vehicles.

High Strength Weight Reduction Materials

The FCVT Program's High Strength Weight Reduction (HSWR) Materials activity focuses on cost-effectively reducing parasitic energy losses due to the weight of heavy vehicles, without reducing vehicle functionality, durability, reliability, or safety. ORNL contributes to the goals of the HSWR activity, which are primarily aimed at applications in Class 8 trucks. These trucks consume more fuel annually than Classes 3 through 7 combined. HSWR activity goals support those of the 21st CTP to reduce the weight of an unloaded tractor-trailer combination from the current 23,000 lb to 18,000 lb by 2012. These goals are to be met so that performance, durability, reliability, and safety characteristics, as well as cost-competitiveness, are comparable to those of conventional vehicle materials. The HSWR activity is pursuing research in numerous technical areas, including cost reduction, design data and modeling, manufacturability, tooling and prototyping, joining and assembly, performance enhancement, and maintenance, repair and recycling. The use of lightweight materials in heavy vehicles presents significant technical challenges to the existing body-assembly joining processes such as resistance spot welding.

At ORNL, researchers are working on the ultrasonic welding process. This is a solid-state joining process and addresses the critical industry need for increased use of lightweight and high-performance materials in heavy-duty vehicles. Initial focus has been on identifying potential applications with industry partners, developing application-specific demonstrations, and fostering technology partnerships. Presently, aluminum, steel and magnesium have been successfully ultrasonically welded. This technique is extremely energy efficient, due to the nature of the solid-state process, and it offers high productivity due to its fast cycle time.

Also in FY 2005, researchers from ORNL and Pacific Northwest National Laboratory (PNNL) began evaluating and designing composite-composite and composite-metal joints. Even when lower-cost carbon fiber becomes available and component processing methods are fully developed, major system design issues will remain where composite materials are joined to other composites and to other metallic materials. In this effort, researchers are developing technically robust and economically attractive joining techniques for attaching a variety of light and heavy materials. Researchers have worked closely with AlphaSTAR to develop and validate an interface between GENOA and the ABAQUS solver, which allows for contact modeling. This is critical for investigating damage in the composite at a bolted joint.

In addition, in FY 2005, a new ASTM standard practice for friction testing was approved and became available for diesel engine designers and manufacturers.

Automotive Propulsion Materials

The FCVT Program's Automotive Propulsion Materials (APM) activity focuses on developing materials technologies that are critical to the 1) advanced power electronics and 2) compression-ignition direct-injection (CIDI) engine and emissions control research areas. The activity supports these two core technology areas by providing materials expertise, testing capabilities, and technical solutions for materials problems. The activity provides component development, materials processing, and characterization to enable successful development of efficient electric drive systems and emissions-compliant CIDI engines.

APM projects at ORNL address materials concerns that directly impact the critical technical barriers in each of the activity's core technology areas mentioned above. These barriers involve fundamental, high-risk materials issues, such as thermal management, emissions reduction, and reduced manufacturing costs.

In FY 2005, a test facility was developed at ORNL to aid designers of automotive components that use permanent magnets to determine how the properties of magnets change as a function of temperature and thermal cycling.

Heavy Vehicle Propulsion Materials

Advanced materials are an enabling technology for fuel-efficient, heavy-vehicle truck engines. Major progress was made in the development of heavy vehicle propulsion materials in FY 2005 including materials for exhaust aftertreatment and materials for air handling, hot section, and structural applications.

The reduction of NO_x and particulate emissions is critically important to the FCVT Program and is highly materials dependent. DOE goals for improved efficiency of heavy vehicles are greatly complicated by engine design and exhaust aftertreatment technologies designed to meet the mandatory EPA emission regulations for 2007 and 2010. Materials and systems research is being conducted to minimize the potentially negative effects of emission-reduction technologies on fuel economy and to result in cleaner and more efficient engines.

ORNL is conducting an integrated effort in diesel engine exhaust aftertreatment, using unique expertise and facilities in ultra-high resolution scanning transmission electron microscopy and high performance computational Density Functional Theory modeling of catalyst behavior to determine the atomic mechanisms of catalyst coarsening and loss of effectiveness in diesel exhaust environments. ORNL is also collaborating with a major diesel engine manufacturer to develop materials analysis tools (X-ray diffraction, Raman spectroscopy, and electron microscopy) for studying catalyst behavior in all stages of the life of the catalyst and determining the parameters that control the life of the aftertreatment device. The lessons learned from these theoretical and experimental observations of catalyst behavior are used as a guide to the development and testing of improved catalyst systems.

ORNL is also collaborating with a diesel engine manufacturer and a domestic supplier of diesel particulate filters to develop an understanding and quantitative model of the durability and expected lifetime of diesel particulate filters. The results of this effort will contribute to the improvement of the filter, development of nondestructive inspection techniques for use during routine engine servicing, and predictions of filter lifetime to facilitate timely replacement.

In a collaborative effort with a domestic automotive company and Lawrence Livermore National Laboratory (LLNL), ORNL is developing an on-vehicle NO_x sensor to enable anticipated exhaust aftertreatment technologies such as the lean NO_x trap and selective catalytic reduction.

Frictional losses in commercial diesel engines represent a significant loss of fuel efficiency. ORNL is developing surface modification technologies to reduce frictional losses in engine components. For example, a simple, low-cost process was developed to greatly improve the frictional behavior of titanium components.

The useful life of engine components can be modeled and predicted via life-prediction testing and modeling methodology developed over the past 20 years by DOE, NASA, and other contributors. ORNL has extended the state-of-the-art life prediction methodology to the microscopic level via the development of copyrighted microstructure-based finite element analysis (FEA) software. The "micro FEA" program uses microstructural images from component materials and commercial FEA codes to predict stresses in components at the microscopic level.

Vehicle Systems

The FCVT Vehicle Systems subprogram at ORNL is principally constituted by simulation and validation projects conducted in conjunction with other national laboratories and industrial partners. ORNL plans to strengthen and increase collaborations with other national laboratories (chiefly ANL) and pursue niche activities that add value to FCVT's systems analysis portfolio.

In FY 2005, ORNL made significant progress in establishing life cycle cost estimation as part of the Powertrain Systems Analysis Toolkit (PSAT), DOE's preferred platform for vehicle systems analytical work. Specific technical accomplishments in this task were highlighted by considerable integration of PSAT and ORNL's Advanced System Cost Model (ASCM). ASCM estimates generic production cost of advanced vehicle configurations, and supplements detailed models at the vehicle subsystem level. Thirteen different light-duty vehicle size classes were studied in FY 2005, with several different powertrain options (including series hybrid, parallel hybrid, fuel cell, etc.). Additionally, a joint ORNL/ANL paper on the cost modeling effort was presented in an international forum (EVS-21) in May 2005. Emphasis in FY 2006 will be on construction of a heavy truck model in partnership with other national laboratories.

Although late in the fiscal year, ORNL re-energized its aftertreatment device modeling effort. This activity has already picked up momentum in the first quarter of FY 2006 and will expand to include advanced combustion modes (e.g., low temperature combustion) and engine configurations (e.g., cylinder deactivation). Researchers at ORNL believe there is exceptionally useful information in the data gathered under the CLEERS project (under the Diesel Crosscut Team) that is not being fully utilized. Early guidance in establishing CLEERS stipulated that the effort was not to produce models, but rather the empirical data from which industry partners and others could build their own models. ORNL and other CLEERS partners have established some "proto-models" which are mathematical expressions of observed behavior (emissions chemistry, etc.). These proto-models have promoted macro-device modeling, and ORNL is proposing further extension of aftertreatment modeling using CLEERS data.

The Heavy Vehicle Drive Cycle project had a new start in FY 2005 and made good progress in initiating the identification of desired information and the necessary on-board sensors, instruments, and data acquisition systems. Significant industry cooperation in commencing on-road cycle runs was obtained as well.

Energy Storage

The Condensed Matter Science Division and the Metals and Ceramics Division of ORNL are collaborating to develop new materials to address some of the key challenges for advanced battery technology. Great progress has been made to improve the lithium-ion battery technology in recent years, but the need for batteries with higher specific energy and power densities, lower cost, safe and robust performance over a 10-year lifetime is particularly acute for the hybrid electric vehicle and full electric vehicle activities.

In FY 2005, research focused on two designs for advanced cathodes for lithium batteries. One of these designs was based on using graphite foam as the support and current collector. The graphite foams developed at ORNL have remarkably high electronic and thermal conductivities that may help alleviate the safety concerns of thermal runaway in lithium-ion batteries. The pore size, density, surface area, and graphitization of the foams can be widely tailored to optimize the electrode performance. Promising results were obtained by coating graphite foam plates with an active battery material, $LiFePO_4$. Continued work will be aimed at developing new synthesis and coating techniques to achieve a thin, uniform coating over the entire surface of the foam. This will be followed by evaluation of thermal management during abuse testing.

The second cathode investigated is comprised of elemental sulfur with copper sulfide as the conductive additive. Others are using carbon black as the additive, but the electrochemical activity and high conductivity of the copper sulfides more than compensate for the added weight. Although tests of these materials fabricated as thin films were promising, significant challenges remain for the design and fabrication of a composite cathode with good structural stability and higher capacity. Continued work on this cathode has been deferred while issues with the lithium anode and electrolyte are addressed.

Investigation of the interface instabilities for the metallic lithium anode is the major new thrust of this project. For electric vehicle lithium-sulfur batteries, the lithium anode must accommodate stripping and plating of several tens of micrometers of lithium in each cycle, at moderate rates. Invariably, the lithium interface with the electrolyte roughens, leading to lost capacity, battery failure, or dangerous reactions. Several years ago, ORNL developed a thin-film solid electrolyte, known as Lipon. This electrolyte forms a stable interface with lithium metal and is quite robust in all solid-state microbatteries. In collaboration with researchers at Hydro Quebec, Lipon films will be assembled with other electrolyte materials in order to stabilize the lithium anode for larger-scale batteries. As part of this effort, new techniques for observing and characterizing the roughening lithium interface will be developed.